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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
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375344

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SEARCH REQUEST FORM

Requestor's Name: BERCH

Serial Number: 09/554077

Date: 3/13/01

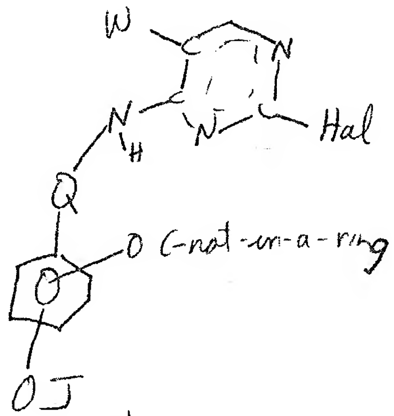
Phone: 4718 (4E12 mb)

Art Unit: 1624 (4D15)

Search Topic:

Please write a detailed statement of search topic. Describe specifically as possible the subject matter to be searched. Define any terms that may have a special meaning. Give examples or relevent citations, authors, keywords, etc., if known. For sequences, please attach a copy of the sequence. You may include a copy of the broadest and/or most relevent claim(s).

W= NH_2 or NO_2



MARY

J = C, but not —(phenyl) ← alc

Q = $(CH_2)_{1-3}$ or $-C(CH_3)(H)-$

Point of Contact:
Mary Hale
Technical Info. Specialist
CM1 12D16 Tel: 308-4258

2 of 2

149.08
149.31

STAFF USE ONLY

Date completed: 3/13

Searcher: Mary

Terminal time: 30

Elapsed time: 36

CPU time:

Total time:

Number of Searches:

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Search Site

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Type of Search

___ N.A. Sequence

___ A.A. Sequence

/ Structure

___ Bibliographic

Vendors

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MM37 STN

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___ APS

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TSCA INFORMATION NOW CURRENT THROUGH July 8, 2000

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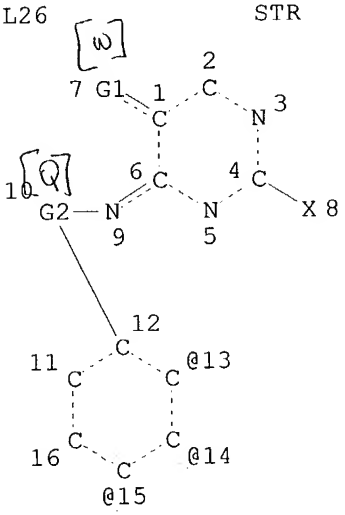
L26 STR



ω= VAR G1=NH2/NO2
Q= REP G2=(1-3) C — open will retrieve $(CH_2)_{1-3}$ or $CH(CH_3)$
VPA 17-13/14/15 U
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 17

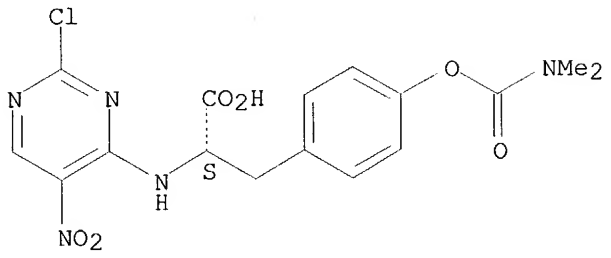
STEREO ATTRIBUTES: NONE
L28 4 SEA FILE=REGISTRY SSS FUL L26

100.0% PROCESSED 57 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.04

L28 ANSWER 1 OF 4 REGISTRY COPYRIGHT 2001 ACS
RN 285140-23-0 REGISTRY
CN L-Tyrosine, N-(2-chloro-5-nitro-4-pyrimidinyl)-, dimethylcarbamate (ester)
(9CI) (CA INDEX NAME)

FS STEREOSEARCH
MF C16 H16 Cl N5 O6
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

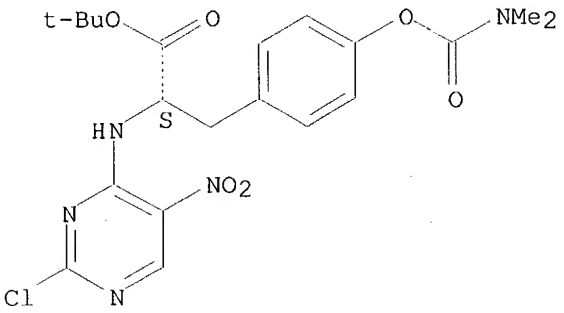
REFERENCE 1: 133:120681 Preparation of amino acid acyl derivatives as inhibitors of leukocyte adhesion mediated by VLA-4. Konradi, Andrei; Pleiss, Michael A.; Thorsett, Eugene D.; Ashwell, Susan; Welmaker, Gregory S.; Kreft, Anthony; Sarantakis, Dimitrios; Dressen, Darren B.; Grant, Francine S.; Semko, Christopher; Xu, Ying-Zi (Elan Pharmaceuticals, Inc., USA; American Home Products). PCT Int. Appl. WO 2000043372 A1 20000727, 342 pp. DESIGNATED STATES: W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US1686 20000121.
PRIORITY: US 1999-PV116923 19990122; US 1999-PV160999 19991021.

AB Disclosed are compds. R2-W:CR1-Q-CR3R3'COX and R2-W'-CHR1-Q-CR3R3'COX [R1 and R2 are joined to form a ring; R3, R3' = H, iso-Pr, -CH2Z or :CHZ, where Z = H, acylamino, alkyl, alkoxy, aryloxy, aryl, aryloxyaryl, carboxy, carboxyalkyl, etc.; Q = O, S, SO, SO2, NH or imino group; W = nitrogen, carbon; W' = nitrogen, carbon, oxygen, sulfur, SO, SO2; X = OH, (un)substituted alkoxy, alkenoxy, cycloalkoxy, cycloalkenoxy, aryloxy, heteroaryloxy or heterocyclyloxy, an amino group] which bind VLA-4. Thus, N-[5-(N-4-toluenesulfonylamino)pyrimidin-4-yl]-L-4-(N,N-dimethylcarbamyloxy)phenylalanine tert-Bu ester was prepd. by condensation of L-4-(N,N-dimethylcarbamyloxy)phenylalanine tert-Bu ester with 2,4-dichloro-5-nitropyrimidine, followed by nitro group redn. and tosylation. Compds. synthesized in the examples are expected to have a binding affinity to VLA-4 expressed by an IC50 of 15 .mu.M or less.

L28 ANSWER 2 OF 4 REGISTRY COPYRIGHT 2001 ACS
RN 285139-31-3 REGISTRY

CN L-Tyrosine, N-(2-chloro-5-nitro-4-pyrimidinyl)-, 1,1-dimethylethyl ester, dimethylcarbamate (ester) (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C20 H24 Cl N5 O6
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



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PRIORITY: US 1999-PV116923 19990122; US 1999-PV160999 19991021.
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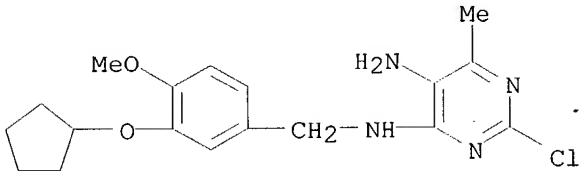
binding affinity to VLA-4 expressed by an IC50 of 15 .mu.M or less.

L28 ANSWER 3 OF 4 REGISTRY COPYRIGHT 2001 ACS
RN 225100-33-4 REGISTRY
CN 4,5-Pyrimidinediamine, 2-chloro-N4-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-6-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H23 Cl N4 O2
SR CA
LC STN Files: CA, CAPLUS



2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 133:350245 Preparation of purine derivative dihydrate as phosphodiesterase IV inhibitor. Sekiya, Kouichi; Takemiya, Akihiro; Ohshima, Masahiro (Mitsubishi Chemical Corporation, Japan). PCT Int. Appl. WO 2000068231 A1 20001116, 29 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (Japanese). CODEN: PIXXD2. APPLICATION: WO 2000-JP2952 20000509. PRIORITY: JP 1999-129499 19990511.

AB Claimed is a dihydrate of 4-[[9-[(3-cyclopentyloxy-4-methoxy)benzyl]-6,8-dimethylpurin]-2-yl-3-oxypropyl]pyridine N-oxide (I); also claimed are : (a) pharmaceutical contg. I as active ingredient; (b) pharmaceutical contg. I as active ingredient for the treatment of asthma, chronic obstructive lung disease and/or other inflammatory diseases; (c) phosphodiesterase IV inhibitor contg. I (d) and intermediates for I. I in vitro showed IC50 of 3.4 x 10-9 M against phosphodiesterase IV, vs. IC50 of 5 x 10-7 M shown by rolipram.

REFERENCE 2: 130:352279 Preparation of purine derivatives as antiasthmatics. This one

Tanaka, Toshihiko; Iwashita, Eiichirou; Tarao, Akiko; Amenomori, Akira; Ono, Yuya (Mitsubishi Chemical Corporation, Japan). PCT Int. Appl. WO 9924432 A1 19990520, 148 pp. DESIGNATED STATES: W: CA, CN, GB, KR, US; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (Japanese). CODEN: PIXXD2. APPLICATION: WO 1998-JP5092 19981112. PRIORITY: JP 1997-310365 19971112.

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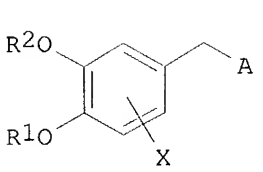

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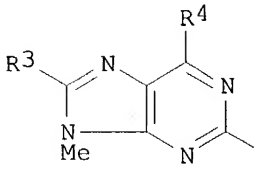
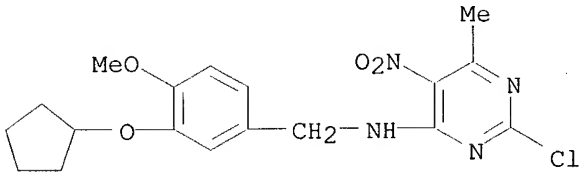


II

AB Title compds. I and II (R1 = alkyl, CHF2; R2 = tetrahydrofuranyl, alkyl, haloalkyl, alkenyl, cycloalkyl, etc.; R3 = H, halo, OH, alkyl, alkoxy, amino, alkylamino, dialkylamino, etc; R4, R5 = H, halo, alkyl, alkoxy, amino, alkylamino, pyrrolidinyl, morpholino, dialkylamino, etc; X = H, halo, NO2) and their salts, useful as antiasthmatics, were prepd. 2-Chloro-9-[(3-cyclopentyloxy-4-methoxy)benzyl]-6,8-dimethylpurine showed IC50 of 6.7 x 10-9 M against phosphodiesterase IV. Formulations contg. title compds. were given.

L28 ANSWER 4 OF 4 REGISTRY COPYRIGHT 2001 ACS
RN 225100-31-2 REGISTRY
CN 4-Pyrimidinamine,
2-chloro-N-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-
6-methyl-5-nitro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H21 Cl N4 O4
SR CA
LC STN Files: CA, CAPLUS



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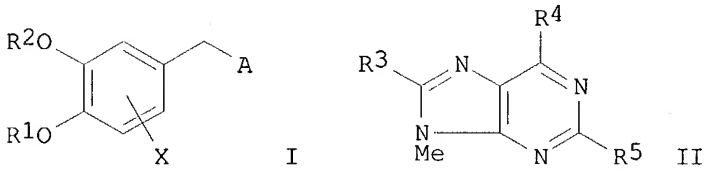
GI



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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	149.08	860.84

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.24	-12.49

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